Title: Safety Applications Project FY18-19 Highlights, FY20 Goals

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Safety Applications Project FY18-19 Highlights, FY20 Goals

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Outline

- Highlights
- Collaborations
- Capabilities
- Infrastructure
- Performance

FY18-19 Highlights

- **David, Laura, and Gopinath joined the team**
- **June 6 ASC Newsbite: MATCH**
- **January 16 ASC Newsbite: SAP→LAP code link**
- **July 31 ASC Newsbite: Code performance improvements**
- **2018 LAAP award**
- **2018 DPoE award:**
  - The Advanced Safety Physics Code Capability Team … improved code quality, capitalized on efficiencies, honed responsiveness to maximize code performance during simulations.

…but the real highlight is seeing our work exercised by users in Safety and Global Security applications.

Collaborations leverage the investment and expertise of others.

- **Trinity COE & CSSE Application Readiness**
  - Pagosa & EOSPAC efficiency improvements
  - ATS2 porting
- **CSEP Data & PEM EOS**
  - EOSPAC efficiency and robustness improvements
- **PEM Explosives**
  - Davis EOS, WSD
- **EAP & CNI**
  - SAP→EAP link
- **LAP & CNI**
  - SAP→LAP link
- **…**

Code capabilities determine the questions that can be addressed using SAP tools.

Past: FY18-19

- SURF+ Reactive Burn
- Davis EOS
- SAP→EAP Link
- SAP→LAP Link
- MATCH
- FLIP+MPM
- Add New Analysis Package
- ParaView

Present: FY20

- aWSD Reactive Burn
- Direct HDF5 Output to an Analysis Package
- FLIP+MPM for HE

Future

- Memory-Efficient STL
- 2D PDV
- 2D Synthetic Radiograph
- DSD
- Improved Brittle Fracture
- Automatic Material Priorities
- Advanced Graphics

Tasks are determined by user need, staff skills, resources, and programmatic constraints.

Infrastructure acts as a force multiplier for software developer skills.

Past: FY18-19

- Confluence Spaces
- Jira Bug Tracker
- Nightly build/test on all Platforms
- Parallel Builds
- Out-of-Source Builds
- Architecture Builds
- Test Coverage
- Performance Logging
- GNU Nightly Testing

Present: FY20

- ATS2 Nightly Testing
- ParaView Dependency
- Compiler Warnings
- Standalone Build/Test
- Relax Intel Floating Point Model
- Resolve Test DIFFs
- Finish LaTeX docs

Future

- Migrate to Git
- Code Release on ATS2
- GPU Support

Paying down infrastructure debt was a major focus of FY18-19.
Most areas are now at par with other projects; some areas exceed.

Improved code performance allows simulations to finish faster or with greater fidelity.

Past: FY18-19

- Inline GD_ES
- Remove EOSPAC Sync Points
- 3D VOF Vectorization
- Windowing

Present: FY20

- Pre-Inverted EOSPAC
- Parallel EnSight Output
- Inline Gen
- Automated Restart
- Physics Robustness
- Improve Interface Efficiency to a Package

Future

- Ray-traced Calico
- Targeted Optimization
- Robustness at Resolution

Implementation, testing, documentation, and user support are not called out—these are our everyday job.

Code Performance

Motivated by the desire for a more realistic test problem, the shaped charge was modified to use tabular EOS.

- **This revealed that EOSPAC dominates execution time, especially for KNL.**
  - Tabular EOS version is 1.4x-4.4x slower than analytic EOS.

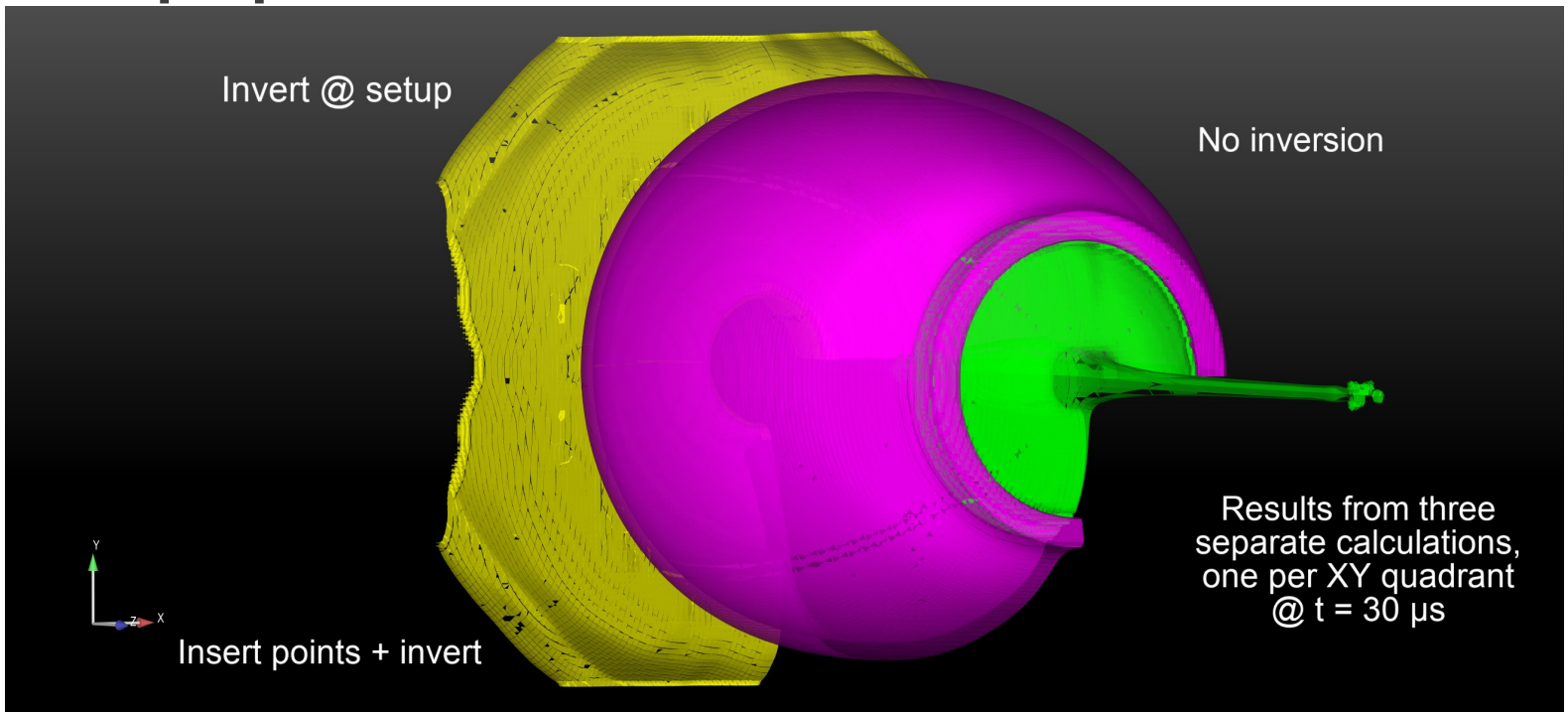
- **In early 2019, EOSPAC 6.4.0 vectorization improvements targeted KNL (Trinity COE, Pimentel).**
  - Team worked through perceived floating point issues in initial deployment.
  - Achieved 2.0x speedup on KNL for PERF_Shaped_Charge nightly performance test.

- **April 2019: Additional ~1.3x speedup across all architectures due to:**
  1. Removing unused debug logic in EOSPAC, and
  2. Removing Pagosa's error check synchronization points after EOSPAC calls.

Performance profiling and coordination across projects contributed to a library improvement that benefits all ASC codes.

Code Performance

As of October 2019, Pagosa can use EOSPAC's invert-at-setup option.

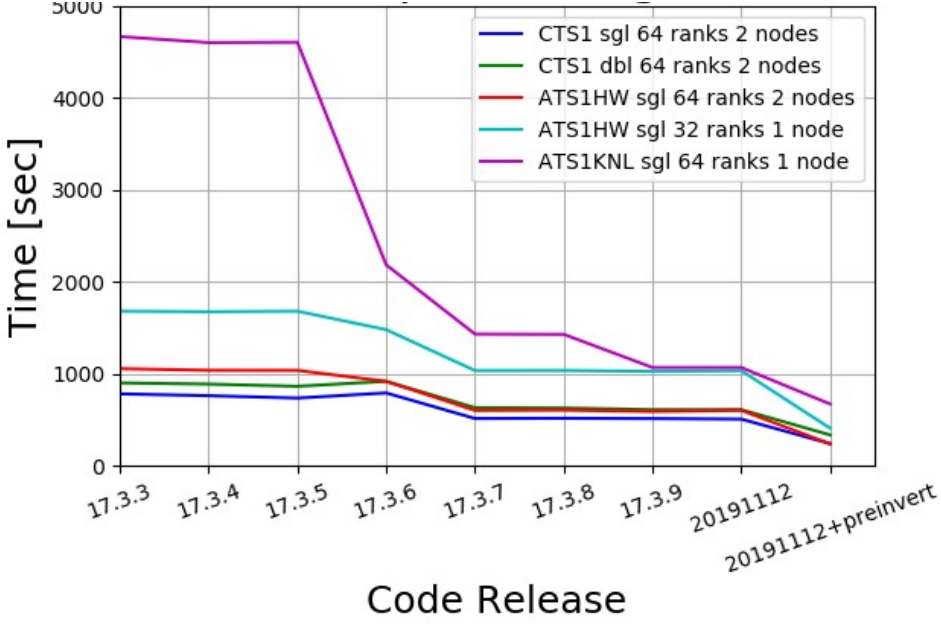


EOSPAC's pre-inverted tables result in a 2.0x speedup on CTS1 & ATS1 with no change in solution quality on Shaped Charge.

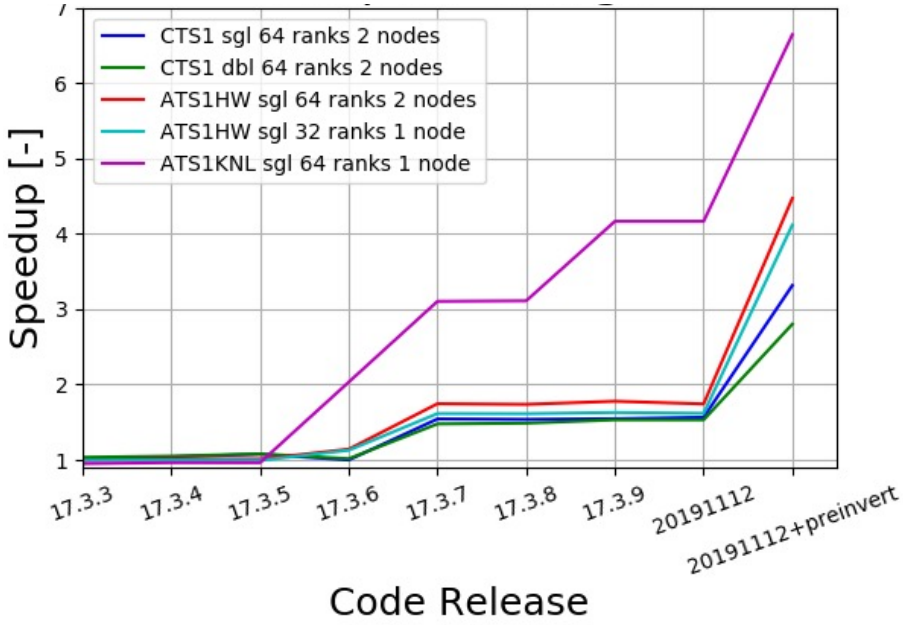
Code Performance

Between November 2018 and December 2019 a 2.8-6.6x speedup in total run time has been demonstrated across all HPC platforms.

PERF_Shaped_Charge is 3D, 814k zones, 64 ranks, 5 materials, 3 analytic EOS, and 2 tabular (EOSPAC) EOS.



The same data are in both plots. Timing is total runtime including Gen, Pagosa, and EnSight output.



ATS1 KNL/HW node-to-node parity was reached in November 2019; this is a significant achievement.